

Amendments to the Claims:

This listing of claims replaces all prior versions and listings of claims in the application:

Listing of Claims:

1. – 36. (Cancelled).
37. (Currently Amended) A computer running a computer program, the computer program executing instructions for performing a method comprising:

receiving information relating to a monoatomic metal ion to be simulated;  
and generating, for observation by a user on a display, a representation of the monoatomic metal ion as a metal molecule by a molecular dynamics simulation, wherein said metal molecule ~~comprises~~ consists of a plurality of metal atoms comprising a center atom and one or more dummy atoms, wherein said center atom has a van der Waals radius greater than zero and has a charge of zero, wherein said center atom is covalently linked to said one or more dummy atoms, ~~and~~ wherein each dummy atom has a positive charge, and wherein said dummy atoms are located at the apices of a polyhedron.
38. (Previously Presented) The computer of claim 37 wherein said dummy atom has a mass of about 0.1 g/mol.
39. (Previously Presented) The computer running a computer program of claim 37 wherein said dummy atom has a mass greater than about 0.1 g/mol.
40. (Cancelled).
41. (Currently amended) The computer of claim 40 ~~37~~ wherein said center atom is

located at the center of said polyhedron.

42. **(Currently amended)** The computer of claim 40 37 wherein said polyhedron is selected from the group consisting of tetrahedron, trigonal bipyramidal, square pyramid, and octahedron.

43. **(Currently amended)** The computer of claim 44 37 wherein said polyhedron is a tetrahedron.

44. (Previously Presented) The computer of claim 37 wherein said metal ion is selected from a main group metal or transition metal.

45. (Previously Presented) The computer of claim 37 wherein said metal ion is selected from the group consisting of zinc, cadmium, mercury, copper, nickel, cobalt, iron, manganese, calcium, and magnesium.

46. (Previously Presented) The computer of claim 37 wherein said metal ion is zinc.

47. **(Currently amended)** The computer of claim 44 37 wherein said metal ion is zinc.

48. (Previously Presented) The computer of claim 37 wherein said metal ion is magnesium.

49. (Previously Presented) The computer of claim 37 wherein said metal ion is calcium.

50. (Previously Presented) The computer of claim 37 wherein said metal ion has a calculated energy of solvation about equal to an experimentally determined energy of solvation for said metal ion.

51. (Previously Presented) The computer of claim 50 wherein said calculated energy of solvation is within about 10% of said experimentally determined energy of solvation for said metal ion.

52. (Previously Presented) The computer of claim 37 wherein said dummy atom has a charge of about + 0.5.

53. (Previously Presented) The computer of claim 37 wherein said dummy atom has a charge of about + 0.3333.

54. (Previously Presented) The computer of claim 37 wherein said dummy atom has a charge ranging from about +0.1 to about +3.

55. - 72. (Cancelled).